



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:41 AM GMT

PDB ID : 2DZD  
Title : Crystal structure of the biotin carboxylase domain of pyruvate carboxylase  
Authors : Kondo, S.; Nakajima, Y.; Sugio, S.; Sueda, S.; Islam, M.N.; Kondo, H.  
Deposited on : 2006-09-27  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

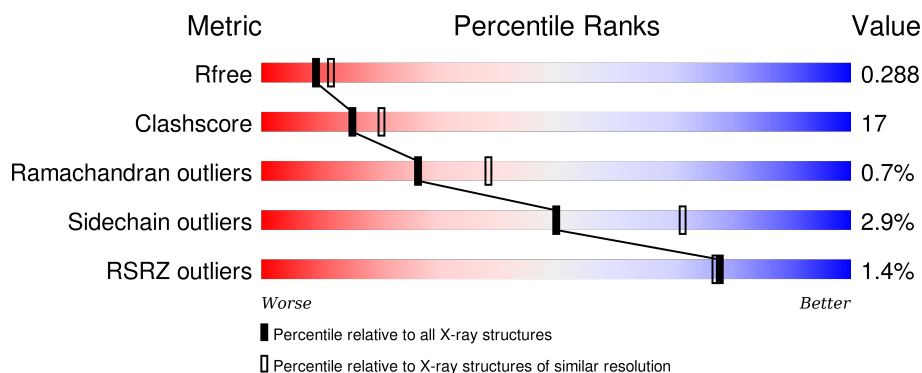
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	461	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>31%</div> <div>.</div> </div> </div>
1	B	461	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>29%</div> <div>..</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7512 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	0	0
			3601	2282	632	675	12			
1	B	453	Total	C	N	O	S	0	0	0
			3562	2258	626	666	12			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	185	Total	O	0	0
			185	185		
2	B	164	Total	O	0	0
			164	164		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.61Å 115.99Å 115.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 19.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.40) 99.4 (19.90-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.82 (at 2.41Å)	Xtriage
Refinement program	CNX2005	Depositor
R, $R_{free}$	0.232 , 0.290 0.232 , 0.288	Depositor DCC
$R_{free}$ test set	2129 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 10.7	EDS
Estimated twinning fraction	0.299 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 42497 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7512	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.34	0/3670	0.52	0/4956
1	B	0.34	0/3629	0.51	0/4899
All	All	0.34	0/7299	0.51	0/9855

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3601	0	3589	130	0
1	B	3562	0	3557	120	0
2	A	185	0	0	6	0
2	B	164	0	0	8	0
All	All	7512	0	7146	248	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (248) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ARG:HG2	1:A:348:ARG:HH11	1.33	0.92

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:ARG:HD3	1:B:106:ILE:HD11	1.51	0.90
1:A:63:GLU:HA	1:A:66:LEU:HD22	1.54	0.88
1:B:349:VAL:HG12	1:B:397:LEU:HD12	1.56	0.88
1:A:275:ASN:HD22	1:A:276:ALA:H	1.25	0.85
1:A:341:ASN:HB3	2:A:610:HOH:O	1.77	0.85
1:A:282:LEU:HG	1:A:291:ILE:HD13	1.57	0.84
1:B:245:GLU:HG2	1:B:300:GLU:HG2	1.61	0.83
1:A:117:MET:SD	1:A:271:VAL:HG11	2.17	0.83
1:B:108:ILE:HG22	2:B:580:HOH:O	1.77	0.82
1:B:316:GLN:HB3	2:B:580:HOH:O	1.79	0.82
1:A:253:SER:HB3	1:A:256:LEU:HB2	1.62	0.82
1:A:19:ILE:HD12	1:A:48:LYS:HG3	1.64	0.77
1:A:7:ARG:HG3	1:B:369:ARG:HD3	1.66	0.77
1:B:170:GLY:H	1:B:173:MET:HE3	1.49	0.75
1:B:161:ILE:HD11	1:B:173:MET:HG2	1.68	0.74
1:A:243:VAL:HG12	1:A:244:VAL:HG23	1.70	0.74
1:B:135:VAL:HG12	1:B:136:ILE:H	1.51	0.73
1:B:69:GLU:OE2	1:B:69:GLU:HA	1.89	0.72
1:B:111:ASN:H	1:B:114:HIS:HD2	1.36	0.72
1:B:108:ILE:CG2	2:B:580:HOH:O	2.34	0.71
1:B:267:LEU:HG	1:B:268:MET:HE3	1.72	0.71
1:B:3:THR:HG23	1:B:4:ARG:H	1.55	0.70
1:B:68:ILE:O	1:B:72:ILE:HG12	1.90	0.70
1:B:135:VAL:HG12	1:B:136:ILE:N	2.07	0.70
1:A:228:HIS:HD2	1:A:230:TYR:H	1.41	0.69
1:B:315:SER:O	1:B:319:ILE:HG13	1.93	0.69
1:B:160:ILE:HG22	1:B:161:ILE:N	2.10	0.67
1:A:248:PRO:HG3	1:A:340:ILE:HD12	1.77	0.67
1:B:270:SER:HB2	2:B:836:HOH:O	1.94	0.66
1:A:160:ILE:HG22	1:A:161:ILE:N	2.09	0.66
1:B:170:GLY:N	1:B:173:MET:HE3	2.11	0.65
1:B:415:LEU:HD13	1:B:437:VAL:HG13	1.77	0.65
1:B:95:GLN:HA	1:B:95:GLN:HE21	1.61	0.65
1:A:136:ILE:HG12	1:A:208:ILE:HD12	1.79	0.65
1:B:3:THR:HG23	1:B:4:ARG:N	2.13	0.64
1:A:258:GLN:HG2	2:A:838:HOH:O	1.96	0.64
1:A:208:ILE:HD13	1:A:289:TYR:CD1	2.32	0.64
1:A:455:THR:OG1	1:A:458:LEU:HD22	1.97	0.63
1:B:256:LEU:O	1:B:260:ILE:HG13	1.99	0.63
1:A:355:LEU:N	1:A:355:LEU:HD12	2.14	0.62
1:B:146:LEU:HD21	1:B:182:VAL:HG12	1.81	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:VAL:HG11	1:B:182:VAL:HG22	1.81	0.62
1:A:227:VAL:HG22	1:A:325:LEU:HD13	1.81	0.62
1:B:161:ILE:HD12	1:B:174:ARG:O	2.00	0.61
1:A:278:THR:HG21	1:A:298:GLN:HE22	1.64	0.61
1:B:237:GLN:C	1:B:452:ILE:HD12	2.20	0.61
1:A:275:ASN:HD22	1:A:276:ALA:N	1.96	0.60
1:B:235:SER:O	1:B:237:GLN:HG3	2.01	0.60
1:B:98:LYS:O	1:B:102:GLU:HG3	2.01	0.60
1:A:19:ILE:HD11	1:A:45:HIS:HA	1.83	0.60
1:A:256:LEU:HD22	1:A:260:ILE:HD11	1.82	0.60
1:B:161:ILE:CG2	1:B:205:GLU:HB2	2.30	0.60
1:A:348:ARG:NH1	1:A:348:ARG:HG2	2.10	0.60
1:A:348:ARG:CG	1:A:348:ARG:HH11	2.10	0.60
1:B:352:GLU:O	1:B:354:PRO:HD3	2.01	0.60
1:A:85:PRO:HB2	1:A:91:SER:HA	1.84	0.59
1:A:160:ILE:HG22	1:A:161:ILE:H	1.66	0.59
1:B:160:ILE:HG22	1:B:161:ILE:H	1.67	0.59
1:A:228:HIS:CD2	1:A:230:TYR:H	2.20	0.59
1:B:245:GLU:CG	1:B:300:GLU:HG2	2.33	0.58
1:A:390:THR:HB	1:A:391:PRO:HD2	1.85	0.58
1:A:114:HIS:HE1	1:A:271:VAL:O	1.87	0.58
1:A:35:ILE:HD12	1:A:55:VAL:HG11	1.86	0.57
1:B:62:ILE:O	1:B:66:LEU:HD13	2.04	0.57
1:B:221:ASP:OD1	1:B:225:ASN:HB2	2.05	0.56
1:A:98:LYS:HG3	1:A:101:ARG:HH21	1.70	0.56
1:A:39:GLU:HG2	1:A:61:PRO:HB3	1.88	0.55
1:B:367:ALA:HB3	1:B:424:ARG:HB3	1.87	0.55
1:A:451:PHE:O	1:A:454:THR:HG22	2.06	0.55
1:B:170:GLY:H	1:B:173:MET:CE	2.19	0.55
1:A:271:VAL:HG12	1:A:271:VAL:O	2.07	0.55
1:B:163:LYS:HE2	1:B:173:MET:SD	2.47	0.55
1:B:163:LYS:HE2	1:B:173:MET:HE2	1.88	0.55
1:B:54:LEU:HD23	1:B:55:VAL:N	2.21	0.55
1:A:215:GLU:CD	1:A:280:GLU:HG2	2.28	0.55
1:A:136:ILE:HG12	1:A:208:ILE:CD1	2.37	0.54
1:A:297:ILE:HD11	1:A:301:HIS:CG	2.42	0.54
1:A:330:VAL:HG12	1:A:332:ILE:HG13	1.88	0.54
1:B:235:SER:HB2	1:B:447:TYR:HE1	1.73	0.54
1:A:57:GLU:HG2	2:A:831:HOH:O	2.07	0.54
1:A:98:LYS:HG3	1:A:101:ARG:NH2	2.23	0.54
1:A:368:TYR:CD1	1:A:423:ILE:HD12	2.43	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ILE:HD11	1:B:173:MET:CG	2.38	0.53
1:A:179:LYS:O	1:A:182:VAL:HG12	2.08	0.53
1:A:187:GLU:HG3	2:A:652:HOH:O	2.07	0.53
1:A:210:ASN:N	1:A:211:PRO:CD	2.72	0.53
1:B:111:ASN:H	1:B:114:HIS:CD2	2.23	0.53
1:A:371:GLY:HA2	1:A:420:GLU:HG2	1.91	0.53
1:B:349:VAL:HG12	1:B:397:LEU:CD1	2.34	0.53
1:A:297:ILE:HG12	1:A:298:GLN:N	2.24	0.53
1:B:188:ARG:O	1:B:192:GLU:HG2	2.09	0.53
1:A:87:TYR:CZ	1:A:299:VAL:HG22	2.44	0.52
1:B:377:ARG:HH11	1:B:377:ARG:HB2	1.75	0.52
1:B:184:GLU:O	1:B:188:ARG:HG2	2.08	0.52
1:B:135:VAL:CG1	1:B:136:ILE:H	2.23	0.52
1:A:305:GLU:HG2	1:A:312:ILE:HG13	1.91	0.52
1:B:307:ILE:HD11	2:B:524:HOH:O	2.09	0.52
1:A:158:TYR:HB3	1:A:159:PRO:HA	1.91	0.52
1:A:146:LEU:HD23	1:A:186:PHE:CD1	2.44	0.52
1:A:237:GLN:O	1:A:452:ILE:HB	2.10	0.51
1:B:190:LYS:HZ2	1:B:201:GLU:N	2.08	0.51
1:A:125:ARG:O	1:A:129:VAL:HG23	2.10	0.51
1:A:36:TYR:O	1:A:54:LEU:HD12	2.10	0.51
1:A:260:ILE:O	1:A:263:ALA:HB3	2.11	0.51
1:B:161:ILE:HG12	1:B:163:LYS:HE3	1.93	0.51
1:A:347:SER:C	1:A:348:ARG:HD3	2.31	0.51
1:B:423:ILE:HD12	1:B:428:THR:HG21	1.93	0.50
1:B:208:ILE:HG22	1:B:211:PRO:HB3	1.94	0.50
1:B:390:THR:HB	1:B:392:TYR:CD1	2.46	0.50
1:B:326:HIS:CD2	1:B:332:ILE:O	2.65	0.50
1:A:275:ASN:ND2	1:A:276:ALA:H	2.02	0.50
1:A:111:ASN:O	1:A:114:HIS:HB2	2.12	0.50
1:A:325:LEU:O	1:A:332:ILE:HB	2.12	0.50
1:B:215:GLU:CD	1:B:280:GLU:HG2	2.31	0.50
1:A:22:PHE:CZ	1:A:34:ALA:HB2	2.47	0.50
1:B:357:ASN:O	1:B:358:PHE:HB2	2.11	0.50
1:B:235:SER:HB2	1:B:447:TYR:CE1	2.47	0.49
1:B:362:THR:HB	1:B:389:ILE:O	2.12	0.49
1:A:179:LYS:C	1:A:181:GLU:H	2.14	0.49
1:A:253:SER:HB3	1:A:256:LEU:CB	2.39	0.49
1:A:152:PHE:HE2	1:A:160:ILE:HD12	1.78	0.49
1:B:297:ILE:HG22	2:B:545:HOH:O	2.12	0.49
1:A:215:GLU:HG2	1:A:280:GLU:HG2	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:LEU:N	1:A:355:LEU:CD1	2.76	0.49
1:B:245:GLU:OE1	1:B:348:ARG:NH1	2.44	0.49
1:B:160:ILE:HG23	1:B:205:GLU:O	2.11	0.49
1:A:347:SER:O	1:A:348:ARG:HD3	2.13	0.49
1:B:267:LEU:HG	1:B:268:MET:CE	2.42	0.49
1:B:354:PRO:HB2	1:B:461:PHE:CZ	2.48	0.48
1:A:82:ALA:HB2	1:A:106:ILE:HB	1.94	0.48
1:A:370:SER:HB3	1:A:421:PHE:CE2	2.48	0.48
1:A:22:PHE:CZ	1:A:49:ALA:HB2	2.49	0.48
1:B:144:ASP:HB2	1:B:148:ASP:OD2	2.14	0.48
1:A:114:HIS:CE1	1:A:271:VAL:HG12	2.49	0.48
1:B:3:THR:CG2	1:B:4:ARG:H	2.19	0.48
1:B:326:HIS:HD2	1:B:332:ILE:O	1.96	0.48
1:B:355:LEU:HD22	1:B:355:LEU:N	2.28	0.48
1:A:144:ASP:HB2	1:A:148:ASP:OD2	2.13	0.48
1:B:69:GLU:CA	1:B:69:GLU:OE2	2.60	0.48
1:A:262:GLU:O	1:A:265:VAL:HG22	2.14	0.48
1:A:150:VAL:O	1:A:154:GLU:HG3	2.14	0.48
1:B:85:PRO:HB2	1:B:91:SER:HA	1.95	0.48
1:B:371:GLY:HA3	1:B:420:GLU:OE1	2.14	0.48
1:B:150:VAL:O	1:B:154:GLU:HG3	2.14	0.48
1:B:135:VAL:CG1	1:B:136:ILE:N	2.76	0.47
1:A:160:ILE:HG23	1:A:205:GLU:O	2.14	0.47
1:A:430:ILE:N	1:A:431:PRO:HD2	2.29	0.47
1:B:163:LYS:HE2	1:B:173:MET:CE	2.44	0.47
1:B:439:HIS:CG	1:B:440:PRO:HD2	2.49	0.47
1:B:160:ILE:CG2	1:B:161:ILE:N	2.76	0.47
1:A:135:VAL:CG1	1:A:136:ILE:N	2.77	0.47
1:A:55:VAL:HG22	1:A:56:GLY:N	2.30	0.47
1:A:334:LYS:NZ	1:A:334:LYS:HB3	2.29	0.47
1:B:11:VAL:HG11	1:B:18:ALA:HA	1.94	0.47
1:A:256:LEU:HD22	1:A:260:ILE:CD1	2.45	0.47
1:B:430:ILE:N	1:B:431:PRO:CD	2.77	0.47
1:A:265:VAL:HG23	1:A:266:GLN:N	2.29	0.47
1:B:389:ILE:N	1:B:389:ILE:HD12	2.30	0.47
1:B:60:LYS:H	1:B:60:LYS:HE3	1.79	0.47
1:A:366:MET:N	1:A:424:ARG:O	2.46	0.46
1:A:19:ILE:CD1	1:A:45:HIS:HA	2.46	0.46
1:A:19:ILE:CD1	1:A:48:LYS:HG3	2.41	0.46
1:A:60:LYS:HB3	1:A:61:PRO:HD2	1.96	0.46
1:B:243:VAL:HG12	1:B:244:VAL:HG23	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LEU:HD13	1:A:150:VAL:HG23	1.98	0.46
1:B:254:ASP:N	1:B:254:ASP:OD2	2.48	0.46
1:A:140:ASP:OD2	1:A:141:GLY:N	2.49	0.46
1:A:74:ILE:HD13	2:A:621:HOH:O	2.15	0.46
1:B:297:ILE:HD11	1:B:301:HIS:CG	2.51	0.46
1:B:183:LYS:O	1:B:187:GLU:HB2	2.16	0.46
1:A:258:GLN:NE2	1:A:262:GLU:OE2	2.49	0.46
1:B:63:GLU:HA	1:B:66:LEU:HD22	1.97	0.46
1:A:133:ILE:HG23	1:A:134:PRO:HD2	1.97	0.46
1:B:152:PHE:HE2	1:B:160:ILE:HD12	1.81	0.46
1:A:215:GLU:CG	1:A:280:GLU:HG2	2.46	0.46
1:A:297:ILE:HG12	1:A:298:GLN:H	1.80	0.45
1:B:160:ILE:CG2	1:B:161:ILE:H	2.29	0.45
1:B:341:ASN:HA	2:B:712:HOH:O	2.15	0.45
1:B:349:VAL:O	1:B:396:LEU:HD12	2.16	0.45
1:A:152:PHE:CE2	1:A:160:ILE:HD12	2.52	0.45
1:A:55:VAL:HG13	1:A:64:ALA:O	2.16	0.45
1:A:160:ILE:CG2	1:A:161:ILE:N	2.77	0.45
1:A:60:LYS:HB3	1:A:61:PRO:CD	2.46	0.45
1:A:174:ARG:HD2	1:A:185:ALA:O	2.16	0.45
1:B:313:VAL:O	1:B:316:GLN:HB2	2.17	0.45
1:B:390:THR:HB	1:B:392:TYR:CE1	2.52	0.45
1:B:35:ILE:O	1:B:35:ILE:HG13	2.15	0.45
1:B:110:PRO:HA	1:B:274:VAL:HG13	1.98	0.45
1:B:228:HIS:HD2	1:B:230:TYR:H	1.63	0.45
1:B:99:ARG:O	1:B:102:GLU:HB2	2.16	0.44
1:A:110:PRO:HA	1:A:274:VAL:HG13	1.99	0.44
1:A:111:ASN:H	1:A:114:HIS:HD2	1.66	0.44
1:A:310:ILE:HA	2:A:692:HOH:O	2.16	0.44
1:B:22:PHE:CZ	1:B:34:ALA:HB2	2.53	0.44
1:A:62:ILE:O	1:A:66:LEU:HD13	2.17	0.44
1:A:36:TYR:O	1:A:54:LEU:HA	2.17	0.44
1:A:160:ILE:CG2	1:A:161:ILE:H	2.31	0.44
1:A:36:TYR:CD1	1:A:46:ARG:HG3	2.53	0.44
1:A:367:ALA:HB3	1:A:424:ARG:HB3	1.99	0.43
1:B:293:VAL:O	1:B:295:PRO:HD3	2.18	0.43
1:A:114:HIS:HE1	1:A:271:VAL:HG12	1.83	0.43
1:A:221:ASP:OD1	1:A:225:ASN:HB2	2.18	0.43
1:B:432:PHE:O	1:B:436:VAL:HG23	2.18	0.43
1:A:128:ALA:HA	1:A:267:LEU:HD13	2.01	0.43
1:A:7:ARG:CG	1:B:369:ARG:HD3	2.43	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:VAL:HG12	1:A:136:ILE:N	2.33	0.43
1:A:231:GLU:OE2	1:A:231:GLU:N	2.42	0.43
1:A:83:ILE:HD12	1:A:100:CYS:SG	2.58	0.43
1:B:16:GLU:HG3	1:B:17:ILE:N	2.34	0.43
1:A:348:ARG:NH1	1:A:348:ARG:CG	2.73	0.43
1:B:4:ARG:HD3	1:B:323:CYS:SG	2.58	0.43
1:B:10:LEU:C	1:B:10:LEU:HD23	2.39	0.43
1:A:422:ARG:O	1:A:423:ILE:HD13	2.19	0.43
1:A:352:GLU:O	1:A:354:PRO:HD3	2.18	0.43
1:B:152:PHE:CE2	1:B:160:ILE:HD12	2.53	0.42
1:A:371:GLY:CA	1:A:420:GLU:HG2	2.48	0.42
1:A:11:VAL:HG11	1:A:18:ALA:HA	2.00	0.42
1:A:297:ILE:HD11	1:A:301:HIS:CD2	2.55	0.42
1:B:9:VAL:HG22	1:B:82:ALA:HB3	2.01	0.42
1:B:170:GLY:O	1:B:172:GLY:N	2.52	0.42
1:A:239:ARG:O	1:A:240:HIS:HB2	2.20	0.42
1:B:100:CYS:HB3	1:B:105:ILE:O	2.20	0.42
1:B:14:ARG:NH1	1:B:393:TYR:CD2	2.88	0.42
1:A:307:ILE:O	1:A:340:ILE:HA	2.19	0.42
1:B:220:GLY:HA2	1:B:225:ASN:O	2.19	0.42
1:B:153:ALA:HB2	1:B:160:ILE:HG13	2.02	0.41
1:B:419:ARG:HE	1:B:419:ARG:HB3	1.70	0.41
1:B:223:GLU:CD	2:B:605:HOH:O	2.57	0.41
1:A:346:GLN:HA	1:A:400:LEU:O	2.20	0.41
1:A:66:LEU:CD1	1:A:66:LEU:N	2.83	0.41
1:A:354:PRO:HG2	1:A:355:LEU:CD1	2.51	0.41
1:B:278:THR:O	1:B:293:VAL:HA	2.21	0.41
1:A:364:LYS:HA	1:A:387:ALA:O	2.20	0.41
1:A:7:ARG:O	1:A:30:ILE:HG23	2.20	0.41
1:A:35:ILE:HA	1:A:53:TYR:O	2.20	0.41
1:A:220:GLY:HA2	1:A:225:ASN:O	2.20	0.41
1:B:237:GLN:O	1:B:452:ILE:HB	2.21	0.41
1:A:8:LYS:HD3	1:A:33:VAL:CG2	2.50	0.41
1:B:355:LEU:CD2	1:B:355:LEU:N	2.83	0.41
1:A:397:LEU:HD12	1:A:397:LEU:HA	1.81	0.41
1:B:163:LYS:HG2	1:B:173:MET:HG3	2.03	0.40
1:B:111:ASN:HB2	1:B:114:HIS:CD2	2.55	0.40
1:B:350:THR:O	1:B:428:THR:HA	2.20	0.40
1:B:299:VAL:HG12	1:B:399:LYS:CD	2.52	0.40
1:A:94:ILE:HD11	1:A:116:ASP:HA	2.04	0.40
1:A:344:ALA:HA	1:A:402:THR:O	2.22	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:ASP:OD1	1:B:426:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	457/461 (99%)	433 (95%)	22 (5%)	2 (0%)	39	56
1	B	449/461 (97%)	421 (94%)	24 (5%)	4 (1%)	21	30
All	All	906/922 (98%)	854 (94%)	46 (5%)	6 (1%)	26	38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	ASN
1	B	171	ARG
1	B	275	ASN
1	A	451	PHE
1	B	172	GLY
1	B	371	GLY

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	381/383 (100%)	369 (97%)	12 (3%)	47	69
1	B	378/383 (99%)	368 (97%)	10 (3%)	54	74
All	All	759/766 (99%)	737 (97%)	22 (3%)	50	71

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	31	ARG
1	A	66	LEU
1	A	183	LYS
1	A	256	LEU
1	A	270	SER
1	A	275	ASN
1	A	334	LYS
1	A	348	ARG
1	A	370	SER
1	A	397	LEU
1	A	458	LEU
1	B	7	ARG
1	B	14	ARG
1	B	60	LYS
1	B	95	GLN
1	B	254	ASP
1	B	347	SER
1	B	348	ARG
1	B	369	ARG
1	B	377	ARG
1	B	443	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	114	HIS
1	A	130	ASN
1	A	228	HIS
1	A	258	GLN
1	A	275	ASN
1	A	298	GLN
1	B	95	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	111	ASN
1	B	114	HIS
1	B	228	HIS
1	B	240	HIS
1	B	326	HIS
1	B	335	GLN
1	B	346	GLN
1	B	356	ASN
1	B	409	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	459/461 (99%)	-0.34	3 (0%) 89 88	15, 23, 37, 44	0
1	B	453/461 (98%)	-0.16	10 (2%) 65 64	15, 23, 50, 73	0
All	All	912/922 (98%)	-0.25	13 (1%) 78 77	15, 23, 41, 73	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	165	ALA	9.7
1	B	172	GLY	5.8
1	B	169	GLY	5.3
1	B	166	LEU	5.0
1	B	168	GLY	4.9
1	B	193	ALA	4.8
1	B	171	ARG	4.5
1	B	170	GLY	3.6
1	A	169	GLY	2.9
1	A	371	GLY	2.5
1	A	140	ASP	2.3
1	B	175	ILE	2.1
1	B	190	LYS	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.



## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.